Introduction to Differentiable Probabilistic Models

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S&P Global

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Primer: Standard Machine Learning

- Usually, we are given a set $\mathcal{D} = \{X, y\}$

$$X = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1m} \\ x_{21} & x_{22} & \dots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nm} \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

where X is our data matrix, and y are our labels.

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  where X is our data matrix, and y are our labels.
- Attempt to fit a model f parameterized by θ with respect to an objective function $\mathcal{L}$

$$\theta^* = \underset{\theta}{\text{argmin}}\ \mathcal{L}\big(f(X;\theta),\ y\big)$$

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- Examples:
  - Classification: Fitting two multinomial distributions
  - Regression: Fitting a Normal centered around the line of best fit

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- Divergences must satisfy 2 properties:
  - $D(P \parallel Q) \geq 0 \quad \forall P, Q \in S$
  - $D(P \parallel Q) = 0 \iff P = Q$

The Kullback-Leibler Divergence

- The KL Divergence for distributions P and Q is defined as:

$$D_{KL}(P \parallel Q) = \int_{-\infty}^{\infty} p(x) \log\left(\frac{p(x)}{q(x)}\right) dx$$

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- Note: the KL Divergence is NOT symmetric:

$$D_{KL}(P \parallel Q) \neq D_{KL}(Q \parallel P)$$

- But we will come back to this later...

Directionality: Forward KL

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$$= \mathbb{E}_{x \sim P}\left[\log\left(\frac{p(x)}{q(x)}\right)\right]$$

Digression: Implementing Expectations

$$
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&= \mathbb{E}_{x \sim P}\left[\log\left(\frac{p(x)}{q(x)}\right)\right]
\end{aligned}
$$

Algorithm 1 $\mathbb{E}_{x \sim P}[f(x)]$

Expectation of $f(x)$ with respect to P

1: $x_1, \ldots, x_n \sim P$ independently

2: **return** $\frac{1}{N} \sum_{x_i} f(x_i)$

Digression: KL to Cross-Entropy

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\end{aligned}$$

Digression: KL to Cross-Entropy

- If we consider $P(y_i = 1|x_i) = p_i$ and $Q(y_i = 1|x_i) = \sigma(f_\theta(x_i))$:

$$\operatorname*{argmin}_\theta D_{KL}(P \parallel Q) =$$

$$\operatorname*{argmin}_\theta -\Big[p_i \log \sigma\big(f_\theta(x_i)\big) + (1 - p_i) \log(1 - \sigma\big(f_\theta(x_i)\big))\Big]$$

- This is the Binary Cross-Entropy Loss

Forward KL: Learning a Normal Distribution (Initial)

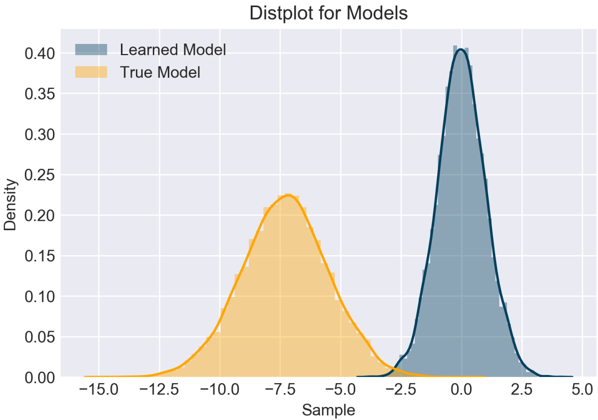
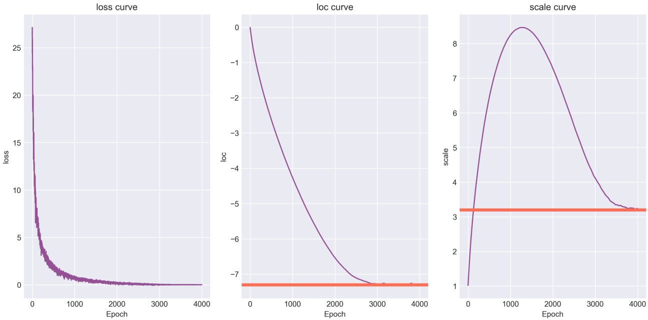


Figure: $P \sim \mathcal{N}(-7.3, 3.2)$, $Q \sim \mathcal{N}(0, 1)$

Forward KL: Learning a Normal Distribution (Results)



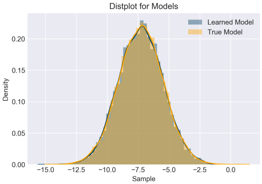


Figure: $P \sim \mathcal{N}(-7.3, 3.2)$, $Q \sim \mathcal{N}(-7.28, 3.24)$

Digression: Gaussian Mixture Models

- We can build a K multi-modal distribution, with weights π, as follows:

$$\begin{aligned} z &\sim \text{Categorical}(\pi) \\ x \mid z = k &\sim \text{Normal}(\mu_k, \sigma_k) \end{aligned}$$

- We can calculate log probabilities by marginalizing out z:

$$\log p(x) = \log \sum_{k=1}^{K} \underbrace{p(z = k)}_{\text{Categorical}} \cdot \underbrace{p(x \mid z = k)}_{\text{Normal}}$$

Digression: Mixture Models (Visual)

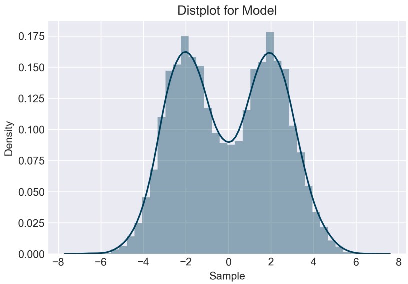


Figure: 2 Mixture Components, Even Weights

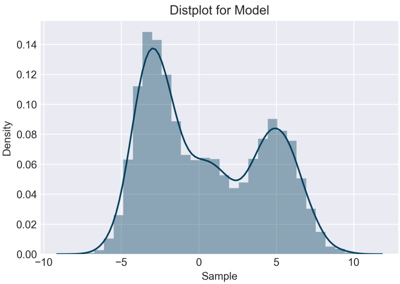


Figure: 3 Mixture Components, Uneven Weights

Forward KL: Learning a Bimodal (Initial)

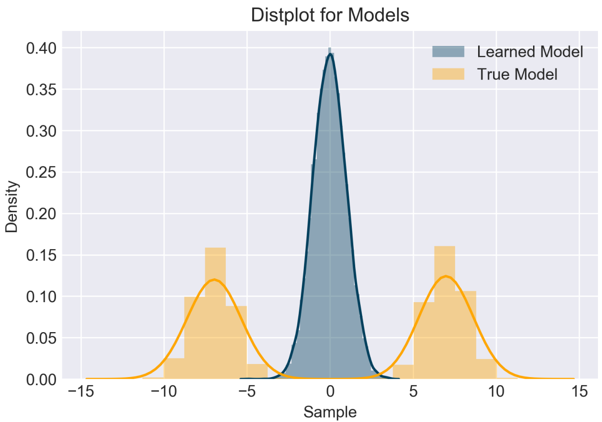


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4),\ \mathcal{N}(7.3, 1.4)\}$
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Forward KL: Learning a Bimodal (Results)

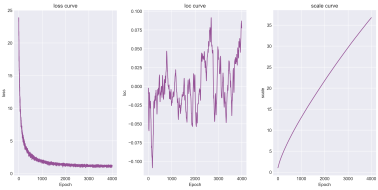

Figure: $Q \sim \mathcal{N}(0.08, 36.76)$

Forward KL: Zero-Avoiding

$$D_{KL}(P \parallel Q) = \int_{-\infty}^{\infty} \overbrace{p(x)}^{\text{Constant}} \log \left(\frac{\overbrace{p(x)}^{\text{Constant}}}{\underbrace{q(x)}_{\text{Variable}}} \right) dx$$

- $p(x)$ is constant-valued, $q(x)$ is variable
- If Q does not support P, then we will sample a point that has a low probability with respect to Q

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- $p(x)$ is constant-valued, $q(x)$ is variable
- If Q does not support P, then we will sample a point that has a low probability with respect to Q
- As $q(x) \to 0$, our loss $D_{KL} \to \infty$
- Hence, the optimal solution is for Q to cover P, i.e. averaging

Forward KL: Loss Landscape

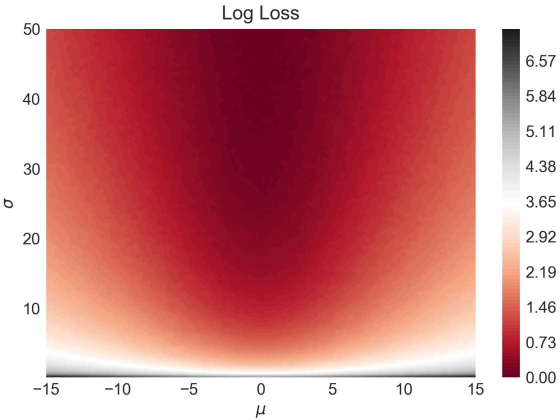

Figure: Loss Landscape for Forward KL Divergence

Directionality: Reverse KL

$$
\begin{aligned}
D_{KL}(Q \parallel P) &= \int_{-\infty}^{\infty} q(x) \log \left(\frac{q(x)}{p(x)} \right) \, dx \\
&= \mathbb{E}_{x \sim Q} \left[\log \left(\frac{q(x)}{p(x)} \right) \right]
\end{aligned}
$$

- The Reverse KL will sample from Q, and evaluate the log probabilities from P and Q
- Recall: KL Divergence is not symmetric, and this has drastic implications...

Digression: Differentiable Sampling via the Reparameterization Trick

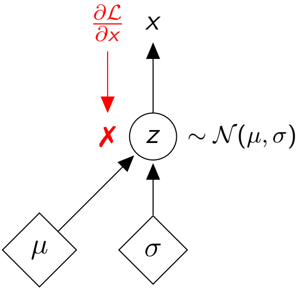

Figure: Original Form

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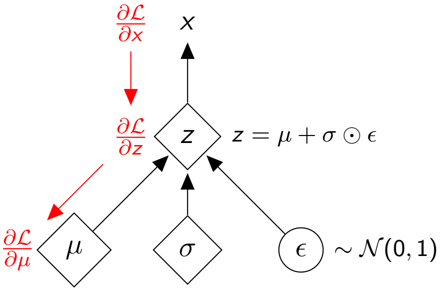

Figure: Reparameterized Version

Digression: Common Reparameterization Tricks

	Reparameterized
$\mathcal{N}(\mu, \sigma)$	$\mu + \sigma \odot \mathcal{N}(0, 1)$
$\mathcal{U}(a, b)$	$a + (b - a) \odot \mathcal{U}(0, 1)$
$\text{Exp}(\lambda)$	$\text{Exp}(1)/\lambda$
$\text{Cauchy}(\mu, \gamma)$	$\mu + \gamma \odot \text{Cauchy}(0, 1)$

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$\mathrm{Laplace}(\mu, b)$	$u \sim \mathcal{U}(-1, 1)$ $\mu - b \odot \mathrm{sgn}(u) \odot \ln\left[-\lvert u\rvert + 1\right]$

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$\mathrm{Categorical}(\pi)$	✗

Reverse KL: Learning a Bimodal (Initial)

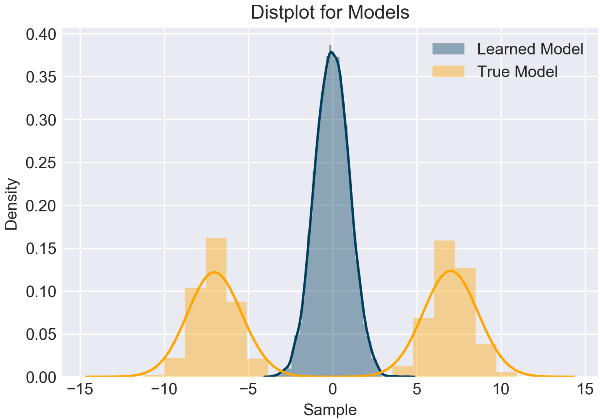
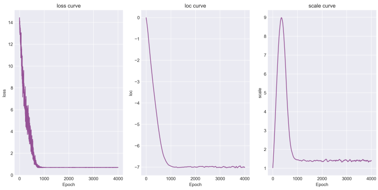


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4),\ \mathcal{N}(7.3, 1.4)\}$
$Q \sim \mathcal{N}(0, 1)$

Reverse KL: Learning a Bimodal (Results)



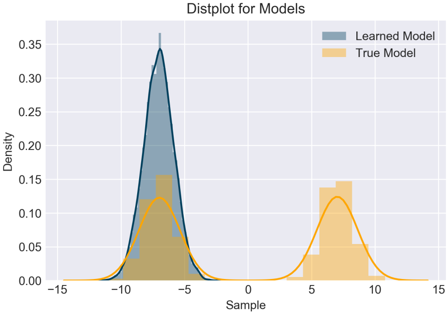


Figure: $Q \sim \mathcal{N}(-7.02, 1.41)$

Reverse KL: Learning a Bimodal Attempt 2 (Results)

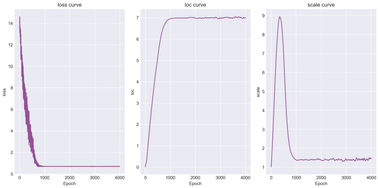


Figure: $Q \sim \mathcal{N}(7.01, 1.46)$

Reverse KL: Zero-Forcing

$$D_{KL}(Q \parallel P) = \int_{-\infty}^{\infty} q(x) \log\left(\frac{q(x)}{p(x)}\right) dx$$

- Unlike the Forward KL, Reverse KL is Zero-forcing
- Why? Because we no longer suffer a penalty from $q(x) = 0$
- However, if $p(x) = 0$, then the optimal value for $q(x)$ is 0
- Result $\implies$ Mode Collapse

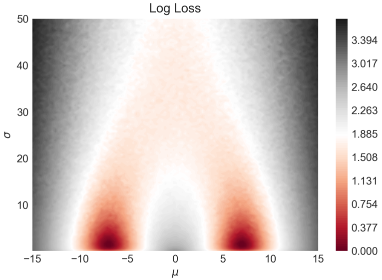


Figure: Loss Landscape for Reverse KL Divergence

Jensen - Shannon Divergence: A Symmetric Divergence

$$\begin{aligned} \text{JSD}(P \parallel Q) &= \frac{1}{2} D_{KL}(P \parallel M) + \frac{1}{2} D_{KL}(Q \parallel M) \\ M &= \frac{1}{2}(P + Q) \end{aligned}$$

- The JS Divergence is a symmetrized version of the KL Divergence
- M is the average of distributions P and Q, and can be represented as a Mixture Model

Jensen - Shannon Divergence: Bimodal (Initial)

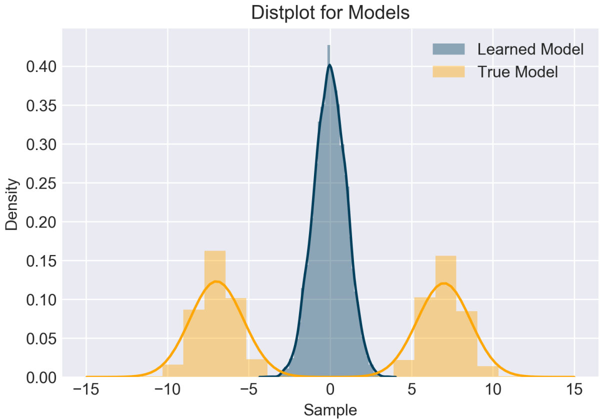


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4),\ \mathcal{N}(7.3, 1.4)\}$
$Q \sim \mathcal{N}(0, 1)$

Jensen - Shannon Divergence: Bimodal (Result)

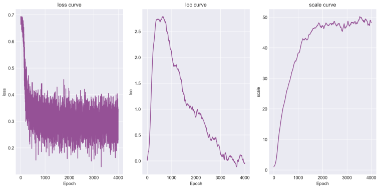


Figure: $Q \sim \mathcal{N}(-0.04, 48.20)$

Jensen - Shannon Divergence: Right Shift (Attempt 2)

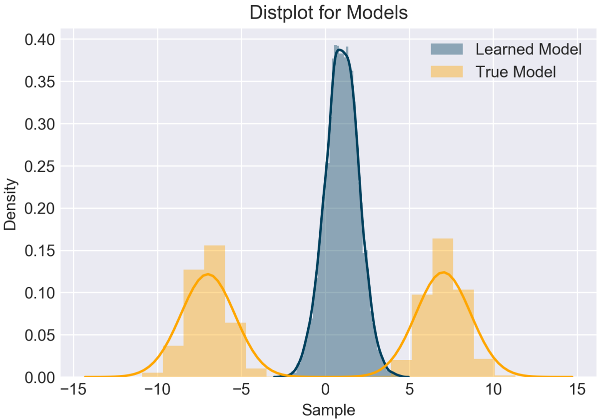


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4),\ \mathcal{N}(7.3, 1.4)\}$
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Jensen - Shannon Divergence: Right Shift (Result)

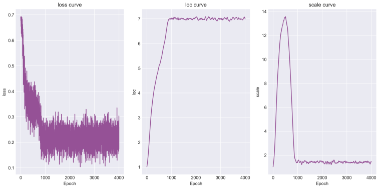
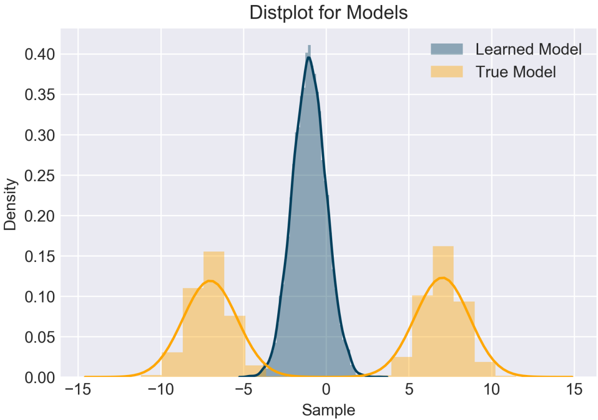


Figure: $Q \sim \mathcal{N}(6.99, 1.43)$

Jensen - Shannon Divergence: Left Shift (Attempt 3)



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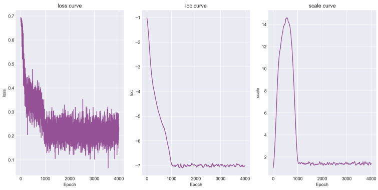
Jensen - Shannon Divergence: Left Shift (Result)



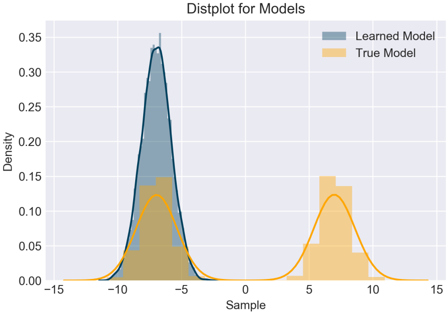


Figure: $Q \sim \mathcal{N}(-6.98, 1.38)$

Jensen - Shannon Divergence Loss

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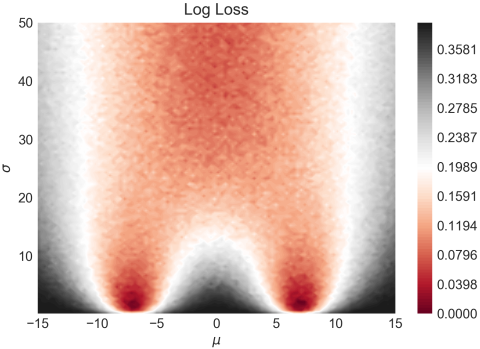

Figure: Loss Landscape for JS Divergence

A Family of Divergences: f-Divergence

- KL Divergence is a special case of the f-divergence
- The f-divergence is a family of divergences that can be written as:

$$D_f(P \parallel Q) = \int \overbrace{q(x)}^{\text{Weight}} f \underbrace{\left(\frac{p(x)}{q(x)} \right)}_{\text{Odds Ratio}} dx$$

A Family of Divergences: f-Divergence

$$D_f(P \parallel Q) = \int \overbrace{q(x)}^{\text{Weight}} \, f\underbrace{\left(\frac{p(x)}{q(x)}\right)}_{\text{Odds Ratio}} dx$$

Divergence	$f(t)$
Forward KL	$t \log t$
Reverse KL	$-\log t$
Hellinger Distance	$\left(\sqrt{t}-1\right)^2$, $2\left(1-\sqrt{t}\right)$
Total Variation	$\frac{1}{2}\lvert t-1\rvert$
Pearson χ^2	$(t-1)^2$, t^2-1, t^2-t
Neyman χ^2 (Reverse Pearson)	$\frac{1}{t}-1$, $\frac{1}{t}-t$

Earth Mover's Distance (Wasserstein-1)

$$W(P,Q) = \inf_{\gamma \in \prod(P,Q)} \mathbb{E}_{(x,y)\sim\gamma}\left[\, \| \, x - y \, \| \,\right]$$

- $\prod(P,Q)$ is the set of joint distributions $\gamma(x,y)$ whose marginals are P and Q
- $\gamma(x,y)$ indicated how much "mass" must be transported from x to y to transform P to Q
- EMD is the "cost" of the optimal transport plan

Summary of Methods

	P		Q	
	$\log p(x)$	$x \sim P$	$\log q(x)$	$x \sim Q$
Cross-Entropy		✓	✓	
Forward KL	✓	✓	✓	
Reverse KL	✓		✓	✓
JS Divergence	✓	✓	✓	✓
f-Divergence	✓	✓	✓	✓

Practical Uses of Divergences

- Forward Kullback-Leibler
  - Maximum Likelihood Estimation
- Reverse Kullback-Leibler
  - Variational Autoencoders
  - Variational Inference
- Jensen-Shannon Divergence
  - Generative Adversarial Network (Original)
- Earth Mover's Distance
  - Wasserstein GAN (WGAN)
- Pearson χ^2 Divergence
  - Least Squares GAN (LSGAN)

Potpourri: Advanced Techniques

	P		Q	
	$\log p(x)$	$x \sim P$	$\log q(x)$	$x \sim Q$
Cross-Entropy		✓	✓	
Forward KL	✓	✓	✓	
Reverse KL	✓		✓	✓
JS Divergence	✓	✓	✓	✓
f-Divergence	✓	✓	✓	✓
Adversarial		✓		✓

Potpourri: Advanced Techniques

1. Transforms
   - Normalizing Flow Models
2. Expectation–Maximization
3. Variational Inference
   - ELBO
4. Adversarial Training (GANs, GANs, GANs)
5. Markov Chain Monte Carlo
   - Metropolis-Hastings
   - Gibbs Sampling
   - Hamiltonian Monte Carlo
   - NUTS